

Statement of Mission Need
for the
Oak Ridge National Laboratory
Multiprogram Computational Data Center Project
Laboratory Infrastructure Division
Office of Science
Non-Major System Acquisition Project

Submitted March 2008

Originator: Johnny O. Moore, Assistant Manager for Science
Organization: ORNL Site Office, Oak Ridge Office
(865) 576-3536

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Mission Need Statement for a Multiprogram Computational Data Center at Oak Ridge National Laboratory

Statement of Mission Need

ORNL is in urgent need of additional infrastructure to accommodate High Performance Computing (HPC). To accommodate this need, ORNL proposes the acquisition by mid-fiscal year 2010 of a multi-program computational data center at ORNL to meet projected schedules for the delivery, installation, and operation of multiple new and very large (petascale growing to exascale) computer systems in a Multiprogram Computational Data Center (MCDC).

The Department of Energy (the “Department” or “DOE”) is a world leader in High Performance Computing. The DOE work in HPC has driven the development of new computing technologies such as vector processing, parallel processing, and now massively parallel systems. For many years, the most powerful computers in the world have been at DOE laboratories. As a priority to the Office of Science, providing ultrascale scientific computing capability is only second to the ITER project (*Facilities for the Future of Science: A Twenty Year Outlook, August 2007*).

In 2004, ORNL was the winner of a Department of Energy Office of Science competition to house a program to provide the world’s most powerful computers in the open scientific community (the “Leadership Computing Facility”). Through this program, a 1-petaflop system will be installed and become operational in the Leadership Computing Facility at ORNL by 2009. With this installation (and others planned for the next 12 to 18 months), ORNL will have depleted its capacity to accommodate new programs. However, ORNL expects that requirements for multiple future DOE–SC petascale systems in the 10 to 250 petaflops range over the next three to four years will lead to an exascale system in the next decade.

Current ORNL computing facilities are capable of supporting the power, space, and cooling requirements of up to 2.5 petaflops computing systems. The MCDC would be capable of supporting envisioned systems on the exaflop capability path - computational capability three orders of magnitude greater than that of the petaflop systems currently scheduled for delivery in fiscal year 2008–2009. ORNL is currently planning to achieve exaflop-level capability for the DOE Leadership Computing Facility in three phases within the next 10 years:

- Phase 1 (2011) will deploy a Cray Cascade system that will be ramped up over a year to deliver 20 petaflops of simulation capability to DOE science missions. This system will already be larger than our present facility can hold and is one of the drivers for an MCDC by mid 2010.
- Phase 2 (2015) will upgrade the central processing units and add accelerator boards to the Cascade system to provide up to 100 petaflops to help solve the next generation of computational grand challenges.
- Phase 3 (2018) will deliver a new 1000-petaflop (i.e., exaflop) system likely to be based on “disruptive” technologies such as three-dimensional chips and optics that are not available today.

Current and future HPC infrastructure needs at ORNL are underpinned by past and future investments by the DOE, the DOD, and the National Science Foundation (NSF). The deployment and operation of these computers are required to solve complex computational problems that the research community deems critical to national security, energy assurance, and the advancement of science. Even the largest existing

HPC systems are insufficient to execute the high-resolution, multiscale, and multiphysics simulations required to model and understand the large-scale, complex physical systems that have greatest interest and greatest potential impact for both science and the nation.

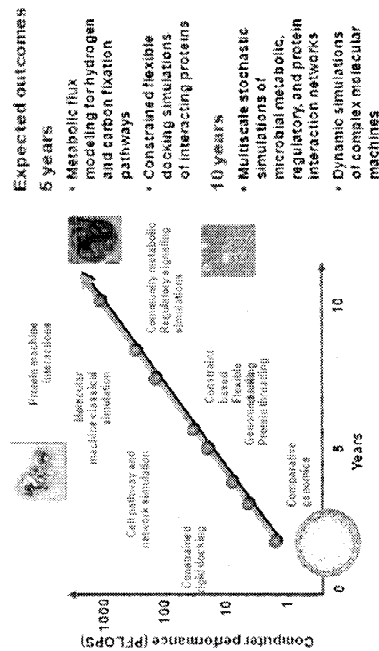
The deployment and operation of these high-performance computers are essential to ORNL's scientific and national security missions. This computational capability supports Basic Energy Sciences (BES), Advanced Scientific Computing Research (ASCR), Fusion Energy Sciences, and Biological and Environmental Research Programs within the Office of Science and other DOE programs. In addition, these computational capabilities support DOD, the Department of Homeland Security and the Department of Commerce national security, climate change and energy assurance programs.

Provided below are charts prepared by the computational science community that depict the dramatically growing computing requirements for solving key problems in nanotechnology, fusion energy, biology, and climate modeling over the next decade. The data show the pressing need for a national facility that can support exaflop computing capabilities in the coming years. ORNL is one of the few locations in the nation that has the potential to field such a facility.

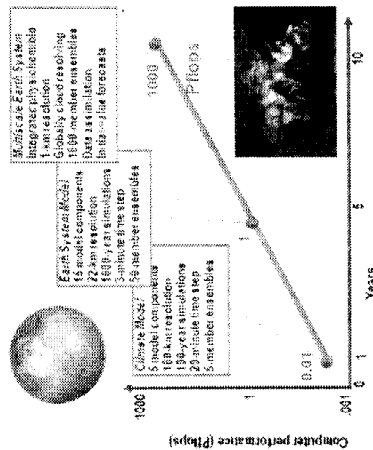
ORNL is uniquely situated among its federal counterparts to lead the expansion of HPC systems. Features unique to ORNL include the following:

- HPC expertise in running very large systems;
- Access to low-cost power;
- High-speed network connectivity;
- Available land to accommodate infrastructure for an exascale facility

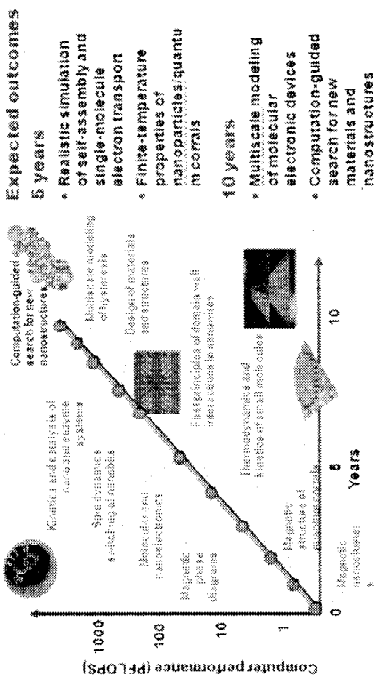
These features will continue to make ORNL attractive for DOE, DOD and NSF and other agency HPC work. Therefore, the MCDC must have the capability to support not only DOE missions but also several other agencies' large-scale computational needs. The mission requirements are such that the MCDC must be configured to accommodate a substantial mix of both unclassified and classified science and national security work. It is anticipated that the installed computer systems will be funded through a combination of DOE and other agency support. ORNL research and development (R&D) staff will be intimately involved in the operation of all systems in the MCDC.



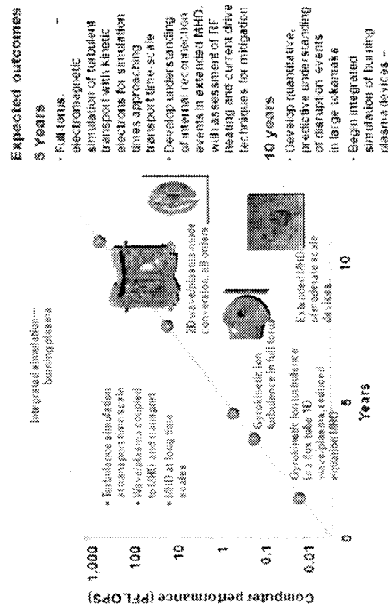
Computational Biology



Computational Chemistry



Nanotechnology



Plasma Energy

Alignment

Program Mission

HPC continues to be one of the fastest-growing programs at ORNL. The large-scale computing capability underpins almost all of ORNL's key scientific disciplines: computational materials science, chemistry, physics, astrophysics, biology, climate research, and applied mathematics. These are just a few examples of scientific fields that depend on HPC for predictive modeling and simulation. The explosive growth of HPC arose through a confluence of growing mission requirements at ORNL from the DOE Office of Science (DOE-SC), NSF, and other federal agencies. ORNL's increased focus on energy assurance and climate change missions is expected to bring additional requirements for very large HPC systems from the Departments of Commerce and Homeland Security.

Strong collaborations have been established between ORNL and the national security community in recent years. ORNL has plans to place additional computer systems in support of certain missions and in support of the High Productivity Computer System (HPCS) program. The HPCS machines are extreme-scale systems, and the first units are due from both Cray and IBM in the 2011–12 time frame. Smaller prototype systems (but still very large by current standards) are very likely to be placed at ORNL in the 2010 time frame to meet mission requirements.

Strategic Fit of Mission Need

DOE has always been the world leader in HPC. Both the National Nuclear Security Administration and DOE-SC have driven the development of new computing technologies such as vector processing, parallel processing, and now massively parallel systems. For many years, the most powerful computers in the world have all been at DOE laboratories. In 2004, DOE-SC competed a program for a Leadership Computing Facility to maintain that leadership and provide the world's most powerful computers to the open scientific community; ORNL won that competition. By 2009, a 1 petaflop system will be installed and operational in the Leadership Computing Facility. This program, coupled with other computing programs now existing or currently planned for ORNL in the next 12 to 18 months, leaves little or no existing space and infrastructure for new programs. New opportunities with HPC currently exist that include multiple future DOE-SC petascale systems in the 10 to 250 petaflops range over the next 3 to 4 years, leading to an exascale system in the next decade.

Working closely with DoD on extreme-scale HPCS systems is a strategic priority for both ORNL and DOE. The nation is making a huge investment in these systems (over half a billion dollars), and ORNL's contributions are absolutely necessary for the overall success of the HPCS program. To this end, DOE is investing \$19.5 million into the HPCS program in fiscal year 2008, has made previous investments, and plans to continue investing until the systems are delivered in the 2011–2012 timeframe. In addition to the funds that DoD has invested through the HPCS program, DoD in fiscal year 2008 will fund a new Extreme Scale Software Center at ORNL to develop the system software, libraries, languages, programming models, and application software for these systems. This center is being supported at ORNL because of the commitment of both DOE and DoD to HPC through the HPCS program.

Priority of Mission Need

DOE is developing plans for expanded computing in the next decade. Current discussions include a major new DOE-SC initiative in exaflops computing by the last half of the next decade. An exaflop computer is 1,000 times more powerful than the computers to be installed at ORNL in 2009. Based on current industry estimates, an exaflop computer is likely to require at least 60 MW of power and 17,000 tons of cooling. Based on the ORNL Leadership Computing Facility 10-year plan, the Laboratory expects to install such a computer system in 2018.

HPCS prototype systems from the DOE/DoD strategic partnership are scheduled to be located at ORNL. In addition, it is highly likely that DOE will place full-scale HPCS machine(s) at ORNL to provide the necessary computing resources for national DOE–SC programs. It is also likely that DoD will place a second system of this type at ORNL to support classified missions. Beyond those systems, the NSF center at ORNL expects to upgrade the systems that ORNL hosts on a path that is similar to the DOE path. ORNL must be in a position to host these machines on schedule.

ORNL's expertise in HPC, computational sciences, and applied mathematics; its ability to quickly, efficiently, and cost-effectively construct facilities that qualify for LEED (Leadership in Energy and Environmental Design) certification with energy-efficient infrastructures; and the availability of plentiful, reliable, relatively inexpensive power from the Tennessee Valley Authority have led other government agencies to ORNL. These agencies are interested in having ORNL host major computer facilities for them. These discussions are urgent, given the current and projected shortfalls of large-scale computer center power, space, and cooling capacity in major urban areas.

The confluence of computing expertise at ORNL and readily available land, power, and water in East Tennessee makes ORNL an ideal location to meet the government's need for facilities to accommodate high-performance computers.

Internal/External Drivers

The major drivers for this project are both classified and unclassified HPC mission requirements from DOE, the Department of Homeland Security, NSF, the National Oceanic and Atmospheric Administration, the Department of Commerce, and other agencies.

Other Drivers

ORNL's collaborative and educational relationships with the NSF and with many universities, especially the University of Tennessee, will be significantly enhanced by the construction of this facility. These relationships have mission execution, long-range educational, and workforce enhancement components. ORNL's capabilities to deploy and support the largest and most powerful computers continue to be a strong attractor of new talent in the HPC field, which is vital for the United States to maintain leadership roles. The availability of a high-level computational work force is also an important factor for economic competitiveness. In addition, continued advances in the largest-scale HPC promise greater efficiencies in design, modeling, and manufacturing that will impact the competitiveness of many industrial sectors across the economy. This facility provides the necessary infrastructure to ensure that ORNL can maintain these capabilities over the foreseeable future.

Capability Gap

Capability Gap

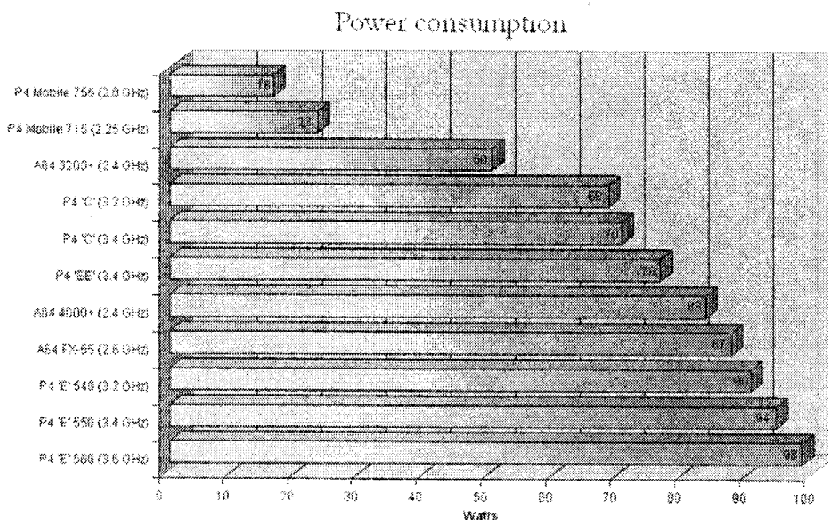
Plans are being implemented for the Leadership Computing Facility and other HPC systems that will fully consume the available power, space, and cooling in the two existing ORNL HPC centers (HPCCs): the Computational Sciences Building (CSB) and the Multiprogram Research Facility (MRF). Over and above these, there are additional requirements for several major new computing systems that are necessary for programmatic science missions, external collaborations, and support of the ORNL information technology/business systems infrastructure. ORNL will not be able to deploy these major new systems within existing facilities starting in fiscal year 2010.

Not only are systems growing larger in size as the Laboratory deploys more powerful petascale systems, but also the power and cooling requirements for individual processors are growing dramatically. The chart on the next page illustrates recent trends showing that the power requirements for individual central processing units will soon surpass 100 watts. Planned systems, comprising tens of thousands and even hundreds of thousands of processors, will require between 10 and 20 MW each of technical power plus additional power for auxiliary electronic storage and cooling.

Even though the present ORNL HPCCs deliver power and cooling at efficiencies that were better than industry norms when they were designed and constructed, they will not have the power, space, or cooling capacity for the larger systems now planned.

Expansion of the infrastructure at existing buildings is possible but not recommended, as these modifications would be substantial and expensive, would result in extended interruptions in HPCC operations, and would adversely affect energy efficiencies. The modifications that would be required include increasing the capacity of the medium-voltage power delivery system and constructing a chilled water plant external to the existing facility. The utility infrastructure expansion would result in elimination of existing office space, a reduction in system availability, reduction of operational efficiency, and increased maintenance requirements.

As computer systems scale up, the sizes of the data sets they produce scale up accordingly. ORNL's classified and unclassified computing operations currently require 5 petabytes of electronic data storage



"CPU power dissipation," Wikipedia at http://en.wikipedia.org/wiki/CPU_power_dissipation

capacity. That is expected to grow to 100 petabytes by 2010 and to an exabyte after that. Considering the anticipated improvements in technology, the space and power required for the expanding storage systems will be more than current ORNL facilities can accommodate without extensive and costly retrofits.

Benefits from Closing the Capability Gap

Constructing an MCDC at ORNL will enable DOE to meet planned and highly potential programmatic computing needs. The MCDC will be available for both DOE-SC missions and other agency missions.

The facility will enable ORNL to successfully meet the requirements of existing programs and to compete for new programs. The continued presence and growth of these programs will significantly enhance DOE's capabilities in all scientific disciplines and will enable ORNL to compete for an increasingly scarce highly technical workforce.

Impact if Gap is Not Resolved

Failure to close the gap will negatively impact the overall ORNL scientific research mission to support DOE, as well as other potential agency missions related to national security. Negative impacts will flow directly to DOE-SC and other major customers who are currently counting on ORNL to provide very large computer systems. If the proposed MCDC is not constructed on the proposed schedule, ORNL will not be able to deploy several planned or potential large-scale HPC systems that are scheduled to come on line starting in mid-fiscal year 2010.

High-Level Interdependences

The MCDC is necessary to support "leadership-class" HPC systems for DOE-SC ASCR and INCITE (Innovative and Novel Computational Impact on Theory and Experiment) programs. Additionally, the MCDC is necessary to support classified systems that are sponsored through various national security agencies and work-for-others programs. Extraordinary advances in computer architecture and software are part of the DOE-SC Strategic Plan for meeting the scientific computation challenges that involve all of its program offices and interagency joint activities. DOE is funding a new computer architecture center to be collocated at ORNL and Sandia National Laboratories to continue the research needed to ensure that the computers will be able to keep up with the mission needs of both the National Nuclear Security Administration and DOE-SC. An inability to provide the appropriate infrastructure for computational needs will impact the efficiency and effectiveness of the DOE-SC science programs at ORNL, which in turn could impact the DOE science mission.

Approach

Planned Approach

The approach used in developing this facility is based on the valuable experience ORNL has gained in constructing, operating, and upgrading new and existing HPCCs to meet the rapidly growing needs of their missions. In a field as dynamic as high-end computing, trying to pinpoint electrical and mechanical demands into the future is virtually impossible. The conventional paradigm of constructing a building and all associated infrastructure as one project is not useful. Therefore, the approach for this project is to construct to the current needs but to plan for and design in the capability for expansion of the power, cooling, and other utilities. The facility will be a scalable data center designed to be completely functional for the first phase of operations. It will be designed for easy, cost-effective and efficient expansion of space, power, and cooling based on mission growth.

Planning, acquisition, siting, designing, building, operating, and maintenance decisions for this facility will be based on the DOE *Guiding Principles for Federal Leadership in High Performance and Sustainable Buildings* under the TEAM Initiative, and will exceed the goals established in Executive Order 13423, "Strengthening Federal Environmental, Energy, and Transportation Management." The project will not seek exemption from the Acquisition Executive for certifying the facility as LEED "Gold." Further, the project will be designed and constructed in accordance with energy-efficiency and energy-conservation requirements as set for in 10 CFR 433, 10 CFR 434, and the related DOE-sponsored Final Rule that was effective January 22, 2008. New equipment and systems will be selected to maximize energy efficiencies and "green" building technologies. The MCDC will be a world leader in data center efficiency; it will be on the leading edge for delivery of power and cooling to data centers.

The MCDC is planned to support classified and unclassified computational science missions. It will be located on approximately 25–30 acres on the ORNL campus. Site development will include roads, utility infrastructure, storage yards, and parking. The facility will have approximately 230,000 gross square feet of total computer space ready to occupy by 2010 to meet mission requirements. An additional approximately 30,000 gross square feet will provide office and utility support space. Construction of 10 MW of technical power and cooling will accommodate the loads forecast for the near term. The capability to place air-handling units below the floor or to provide duct cooling to machine/machine clusters will be provided. The computer room square footage will have the capability to be divided between classified and unclassified computing.

Computer room power and cooling infrastructure will be timed and tailored to the specific mission requirements. These capacity increases will include state-of-the-art technological advances of their own. This “just-in-time” philosophy will provide the most sustainable building, most efficient power and cooling, and most current energy recovery techniques in sync with providing the most efficient and advanced computers.

Once this mission need is approved, the acquisition strategy will fully explore all business case alternatives for delivery of the MCDC identified in the preliminary engineering study, which include: do nothing (base case), construct a new building, lease space either off site or in alternatively financed new construction on site, or renovate an existing building on site to ensure project delivery of facility and infrastructure by due dates established by the mission need.

Assumptions

The project is based on the continuation of the methodology used for data centers previously built at ORNL. This approach incorporates Lessons Learned and energy conservation measures from these previously constructed new and upgrade projects. This approach is to keep program costs as low as possible to while still meeting mission requirements.

The total area for this facility is planned to be approximately 260,000 gross square feet. The data center will have adequate power and cooling for near-term missions in 2010, and the facility and facility infrastructure will be capable of expansion of power and cooling as future missions require.

The acquisition strategy is based on the current evaluation of the following alternatives:

1. No Action: This alternative fails, as mission need cannot be accomplished. The current growth of large-scale computing needs is at a rate that precludes the option of retiring/replacing older systems in sufficient time to accommodate new systems in existing facilities. This would jeopardize the ability to deliver several planned large-scale HPC systems scheduled for mid-2010.
2. Line Item to Construct a New Facility: This alternative will address the need through a line item construction project.
3. Leasing: This alternative will evaluate leasing suitable space within close proximity to the site and leasing space in an alternatively financed facility constructed on the site.
4. Line Item to Renovate an Existing Facility(s): This was the initial approach considered. Extensive data were evaluated with regard to renovating a facility previously used for computing services in Building 4500N at ORNL. The overall need would require renovation of four to five wings and an expansion of the infrastructure in the adjacent areas. This alternative likely would fail to meet mission need because of the estimated cost of renovation (as detailed in earlier estimates to upgrade the facility to improve laboratories and office space), the lack of operational space for occupants during the renovation, the high risk and cost of upgrading unsuitable existing infrastructure (power, water, and cooling) in a highly congested area, the cost of bringing in the power feeds from the remote

substations, and the protracted schedule for renovation (it would take 10 years to accomplish in a phased approach).

The following criteria or factors are considered for evaluation and comparison in the alternative analysis and acquisition planning:

- life-cycle cost
- reasonableness of schedule
- ability to meet functional requirements and operational efficiencies
- other assumptions and constraints
- best value to government of proposed alternative

Constraints

This project will provide a new expanded computing capability. For the purpose of establishing a funding profile, a cost range of \$55 to \$65 million is used as the basis for the resource requirements and schedule, based on the results of recent engineering studies and parametric estimates of the various site considerations.

Risks

The risks anticipated during implementation of the proposed facilities are typical of standard commercial building design and construction. Facility design technology and construction methods for this type of facility exist and will be used. An essential part of the early project planning will be to ensure all potential risks associated with this project have been identified, analyzed, and mitigated via an effective project risk management plan. An adequate contingency reserve will be provided for these risks.

Technical Risks

ORNL has developed other HPC facilities during the past 5 years and has considerable experience in the design, construction, and operation of these facilities. It will apply Lessons Learned to the development of the MCDC. A technical study of alternative sites considered various technical risks, although no significant risks were identified. All equipment and construction work in the project involve technology based on conventional, industrial standards and construction practices. No unusual technical or research and development requirements or constraints are known to exist that would hinder the design and construction of a new computing facility and the schedule. A risk that this project will mitigate is that of building a facility to accommodate computer technology that becomes outdated, or overbuilding a facility in anticipation of technology to be available in 2 to 5 years, which, by the time it is ready to be installed, has changed so drastically that the facility is no longer compatible with it or has to be substantially modified to accommodate it. Natural phenomena hazards have been considered and do not pose a risk.

Safety Risks

Environmental, safety, and health issues during construction of the proposed facilities are typical of standard industrial building construction. No unusual demolition and decontamination activities are anticipated. Sites having lower potential for alteration or disturbance of the natural or biologically sensitive environment on or around the proposed facility will be considered. The facility is to support classified and unclassified computational sciences missions. Thus, although the site will have public areas, property protection areas and surrounding areas of the proposed facility shall comply with ORNL security requirements. Appropriate safeguards and security measures—such as distance from main roads, berming, and a large site to accommodate special barriers—will be considered during project planning and conceptual design to minimize any security risk or vulnerability. A risk assessment will be performed for the development of the MCDC prior to project implementation.

Cost Risks

There are no foreseen significant cost risks, as the project is conventional design and construction with a duration of 15 to 18 months, if renovation or building a federally funded facility is not selected as a viable alternative. The acquisition planning and alternatives analysis ("Business Case") will identify any risks. Provision has been made for material and labor escalation in the cost basis. A study was completed analyzing various sites and the costs to develop each site. Based on preliminary estimates of each site considered, a 25% contingency has been included in accordance with DOE cost-estimating guidelines.

Schedule Risks

No schedule risks are foreseen, as the project is conventional design and construction; schedule contingency is included in the baseline schedule, if renovation or building a federally funded facility is not selected as a viable alternative. The Business Case will identify any risks. Completion of planned construction in 2010 depends largely on prompt resolution of the Business Case.

Legal Risks

There are no known legal risks, as the project will be designed and executed in accordance with current applicable public laws, codes, standards, DOE Orders, and best management practices.

Resource and Schedule Forecast

Estimated Cost

The project plan is to start operation with large-scale HPC systems that are scheduled to come on line in mid-2010. Therefore, design must be completed by the end of fiscal year 2008 and construction initiated in early 2009.

The conceptual cost profile in Table 1 has been estimated for planning purposes only. A definitive profile and schedule will be established during conceptual design. The total project cost range can be expected to change when the conceptual design is completed. Changes to the proposed schedule will impact the cost profile.

Table 1. Cost profile

	Build a new facility	Renovate an existing facility*	Lease an offsite facility**
FY 2008	\$ 5M	\$ 10M	N/A
FY 2009	\$40M	\$ 65M	N/A
FY 2010	\$15M	\$ 30M	N/A
Total	\$60M	\$105M	N/A

**Assumed to be accomplished in 3 years if there are no issues related to relocating staff during the renovation. This is a conservative estimate. If the schedule were a more realistic 10-year renovation project, costs would be approximately 3x*

***If facility is leased, hard costs are assumed to be slightly less than for a line item. However, no capital expenditures are incurred. Lease payments would begin at substantial completion.*

Estimated Schedule

Table 2 shows the preliminary milestone schedule for Critical Decisions. For the purpose of the mission need analysis, the following preliminary schedule is based on projected schedules for the delivery, installation, and operation of multiple petascale/exascale computer systems.

Table 2. Preliminary schedule dates

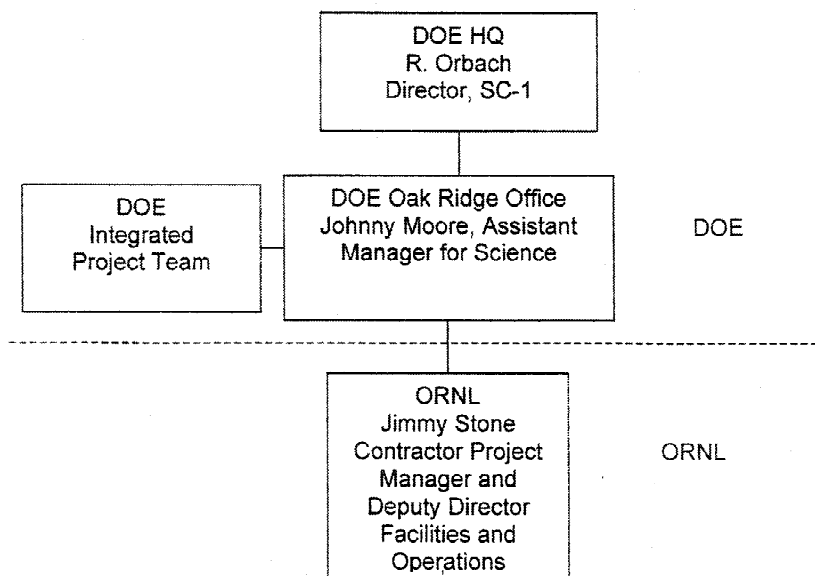
CD-0 Approve Mission Need	2nd quarter FY 2008
Start Design	3rd quarter FY 2008
Start Construction	1st quarter FY 2009
Start Operations	1st quarter FY 2010

Project Structure and Organization

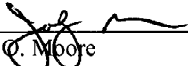
The approach for project organization and structure is highly dependent on the acquisition strategy. At the minimum, to the point of Acquisition Strategy approval, the Assistant Manager for Science at the ORNL Site Office, will serve as the acquisition executive. The acquisition strategy is proposed to be signed by the DOE Under Secretary of Science. The Federal Project Director, with the support of the DOE-ORO Office of the AMS, will provide overall project management oversight, approve key project documents, and provide necessary funds via approved financial plans. UT-Battelle will furnish engineering support, including the procurement documentation and management support services, and will administer construction subcontracts and construction inspection.

The project team will include those listed on the chart below. Membership will be revised and expanded as necessary as the project matures. The appropriate stakeholders (including users) and utility and facility operations managers will be part of the integrated project team.

The acquisition and all other project execution processes will be effectively managed using a tailored approach commensurate with the risk, complexity, cost, and schedule factors of this project and consistent with approved systems and procedures. A project execution plan will be developed.



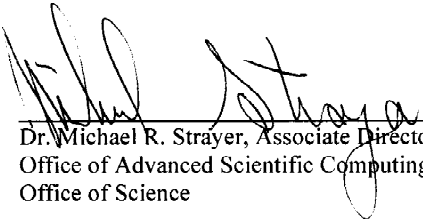
Submitted by:


Johnny O. Moore
Federal Project Director
Assistant Manager for Science,
Oak Ridge Office

3/5/2008
Date

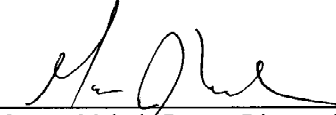
Recommendations:

The undersigned "Do Recommend" (Yes) or "Do Not Recommend" (No) approval of CD-0, Approval of Mission Need, for the **Oak Ridge National Laboratory Multiprogram Computational Data Center Project** as noted below.


Dr. Michael R. Strayer, Associate Director
Office of Advanced Scientific Computing Research
Office of Science

Date

Yes ☒ No ☐


George Malosh, Deputy Director for Field Operations
Office of Science

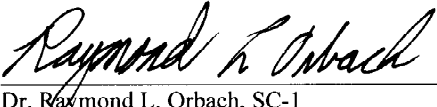
Date

3/7/07

Yes ☒ No ☐

Approval:

After reviewing the project justification material, including the positive recommendation from the Office of Advanced Scientific Computing Research, I find the Statement of Mission Need for the Multiprogram Computational Data Center project satisfactory and authorize DOE-ORO AMS to proceed with CD-0.


Dr. Raymond L. Orbach, SC-1
Under Secretary for Science

Date

March 14, 2008